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Institute of Mathematical Sciences
Division of Electromagnetic Research

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Modification of Effective Range Theory in the Presence of a Long-Range ($1/r^4$) Potential

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Thomas F. O'Malley, Larry Spruch, and Leonard Rosenberg

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ABSTRACT

For short range potentials, there exists the effective range theory expansion $k^{2L+1} \cot \eta(L) = -1/A(L) + \frac{1}{2} r_o(L) k^2 + \ldots$, where $\eta(L)$ is the phase shift for angular momentum L. For long range potentials, (potentials which vanish at large r only as some power of $1/r$), an expansion in k^2 does not exist. For $V(r) \to \text{const} \times r^{-n}$ for $r \to \infty$, the term at which the expansion breaks down depends upon L and upon n; $A(L)$ cannot be defined if $n \leq 2L + 3$ while for example for $L = 0$ one cannot define r_o in the usual way if $n \leq 5$.

A detailed study is made of the case $n = 4$. This case is of considerable interest since it arises, in the adiabatic approximation, in the scattering of a charged particle by a neutral polarizable system; the present analysis is concerned with the scattering by a static potential, but it can be readily generalized to include scattering by a compound (polarizable) system. The analysis is very much simplified by the existence of known mathematical solutions, Mathieu functions, of the Schroedinger equation with $V(r)$ equal to $\text{const} \times r^{-4}$. The expansion of $k \cot \eta(0)$ about $E = 0$ contains a number of terms not present in the usual effective range theory, including a term linear in k. The expansion about the energy of a weakly bound state does not contain these additional terms. It is rather of the usual form, but the correction will be of lower order than k^4. The leading terms in the expansion of $k^2 \cot \eta(L)$ for $L \neq 0$ are also obtained.

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1. INTRODUCTION

Effective range theory[1,2], which gives the leading terms in the expansion of k^{2L+1} cot $\eta(L)$ as a function of the energy, where $\eta(L)$ is the scattering phase shift for angular momentum L, has been a very important tool in the analysis and interpretation of low energy nucleon-nucleon scattering data. Restricting ourselves for the moment to the value L = 0, it will be recalled that for neutron-proton (or neutron-neutron) scattering, one expects the shape independent approximation[3]

$$k \cot \eta(0) \sim - 1/A + \tfrac{1}{2} r_o k^2 \qquad (1.1)$$

to be a useful one for $k \lesssim k_{MAX}$, where, roughly, $k_{MAX} r_o = 1$. In Eq. (1.1), $A \equiv A(0)$ is the scattering length and $r_o \equiv r_o(0)$ is the effective range. For neutron-proton scattering, a characteristic length is of the order of 10^{-13} cm, as is in particular r_o, and one therefore expects the shape independent approximation to be useful for energies up to perhaps 10 Mev.

The range of validity of effective range theory must to some extent be reexamined in each new application. Nevertheless, in atomic physics, one might well expect to have $r_o = t\, a_o$, with t a number somewhat greater than 1 and a_o the Bohr radius; one might further expect that the range of validity of the theory would again be given by $k \lesssim 1/r_o$. Effective range theory would then be quite useful[4]. For the scattering of an electron by an atom, for example, the theory would be useful from zero energy up to energies of the order of $\hbar^2/(2mr_o^2) = (13.6/t^2)$ev; for t not too large compared to unity, this interval is one of the most interesting portions of the energy spectrum.

In point of fact, the situation in atomic scattering processes is rather more complicated than indicated so far. It is the purpose of the present paper to show that r_o as normally defined is infinite, and that the very form of effective range theory must be modified for the atomic case[5]. The origin of the deviation from the normal form lies in the fact that while it is not always explicitly stated, the usual effective range theory assumes that the potentials are of short range, while the effective potentials of atomic scattering theory are of long range. We will refer to a potential as of short range if it falls off faster than any power of $1/r$. Thus, in effective range theory for short range potentials and for angular momentum L, one shows that there exists the expansion

$$k^{2L+1} \cot \eta(L) = -1/A(L) + \tfrac{1}{2} r_o(L)k^2 + O(k^4). \qquad (1.2)$$

It is very well known, however, than an expansion of this form is not always valid. For a potential which asymptotically approaches a Coulomb potential, the very definition of phase shift must be altered; the extension of effective range theory to include this case was given some time ago.[1,2] More significantly, for a repulsive potential which is everywhere proportional to $1/r^2$, a phase shift does exist but is energy independent so that for all positive k, and for all L.

$$k^{2L+1} \cot \eta(L) = C(L)k^{2L+1}. \qquad (1.3)$$

Eq. (1.3) is an identity, not the leading term of an expansion, and is clearly not of the form of Eq. (1.2).

Now for small energies the effective potentials of atomic physics do not fall off faster than any power of $1/r$. Thus, the interaction with a neutral molecule (which does not have a permanent dipole moment) of an

ion of charge Ze and of sufficiently small energy behaves asymptotically as

$$V(r) \to -\tfrac{1}{2} Z^2 e^2 \alpha / r^4 \qquad \text{for } r \to \infty, \tag{1.4}$$

where α is the molecular polarizability, and r is the distance between the centers of the ion and of the molecule. For an electron or positron rather than an ion, one need merely replace Z^2e^2 by e^2. (It is rather more difficult to justify the adiabatic approximation in the scattering of electrons or positrons by molecules than in the scattering of ions by molecules, but it is nevertheless almost certainly a valid approximation at sufficiently low energies.) One then finds for all $L > 0$ that cot $\eta(L)$ is proportional to k^{-2} and hence that k^{2L+1} cot $\eta(L)$ is proportional to k^{2L-1} for sufficiently small values of k. Thus, even the leading term in the above expansion, Eq. (1.2), is incorrect for $L > 0$ when a long range $1/r^4$ polarization potential is present. The leading term in k cot $\eta(0)$ is independent of k for the polarization potential, as it is for short range potentials. The next term, however, is <u>not</u> proportional to k^2, as we shall see, so that the shape independent approximation is not valid even for $L = 0$.

The problem which motivated the present research is the problem of the scattering of an electron or an ion by a neutral molecule which does not have a permanent dipole moment. The asymptotic $1/r^4$ dependence of the effective interaction that is generally assumed for that case, at low energy, is a consequence of the adiabatic approximation. Though some doubt has recently been cast on the validity of this approximation, we believe it to be basically correct. However, in the present paper that question will not be tounched upon. In order to avoid the additional

difficulties that are introduced in the analysis of scattering by compound systems, (the difficulties are complexities rather than questions of principle), we will restrict our attention to the mathematical question of the appropriate form of effective range theory for scattering by a static central potential which obeys the usual requirements for small values of r and which approaches $-\frac{1}{2} Z^2 e^2 \alpha / r^4$ for large r. Applications to physically interesting problems will be considered in a subsequent paper.

Section 2 will consider the origin of the breakdown of the expansion of $k^{2L+1} \cot \eta(L)$ as a power series in k^2 for long range potentials. The rest of the paper is primarily concerned with the polarization potential which goes asymptotically as a multiple of $1/r^4$. In Section 3, we consider in some detail the solutions of a Schroedinger equation with a potential which is everywhere proportional to $1/r^4$. These solutions play the same role as do the free solutions in the usual formulation of effective range theory. The subsequent sections develop expansions of $k^{2L+1} \cot \eta(L)$ about $E = 0$, and, for $L = 0$, about the energy of a bound state.

2. BREAKDOWN OF POWER SERIES EXPANSION OF $k^{2L+1} \cot \eta(L)$ FOR LONG RANGE POTENTIALS

A - Conditions for existence of A(L)

Before proceeding to an analysis of the long range $1/r^4$ polarization potential which is our primary concern, we will attempt to obtain some insight into the general question of the origin of the breakdown of the expansion of $k^{2L+1} \cot \eta(L)$ as a power series in k^2.

The wave function u(r) to be determined is defined by the Schroedinger equation

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{L(L+1)}{r^2} - \frac{2\mu}{\hbar^2} V(r)\right] u(r) = 0 \qquad (2.1)$$

and by the appropriate boundary conditions. For short range potentials, $V(r)$ can be neglected entirely for very large r and $u(r)$ must there approach a linear combination of the free solutions; we can therefore impose the boundary conditions

$$u(0) = 0,\ u(r) \to k^L\left[\cot\eta(L)\, kr j_L(kr) - kr n_L(kr)\right] \text{ for } r \to \infty\ . \qquad (2.2)$$

For $k = 0$, $u_o(r)$ should approach a linear combination of the $k = 0$ free solutions, r^{L+1} and r^{-L}. If in Eq. (2.2) we let $k \to 0$, and if further we use

$$\lim_{k\to o} k^{2L+1} \cot \eta(L) = -1/A(L), \qquad (2.3)$$

we do in fact find that for $r \to \infty$ we have such a linear combination, namely,

$$u_o(r) \to (2L-1)!!\ r^{-L} - r^{L+1} / \left[(2L+1)!!\ A(L)\right], \qquad (2.4)$$

where

$$(2L-1)!! \equiv 1 \times 1 \times 3 \times \ldots (2L-1),\ (2L+1)!! \equiv 1 \times 3 \times 5 \times \ldots (2L+1).$$

We of course also have $u_o(0) = 0$. The terms which were dropped in Eqs. (2.2) and (2.4) are terms which fall off with r faster than any power of $1/r$.

For <u>long</u> range potentials, however, $u_o(r)$ will <u>not</u> have the asymptotic form specified by Eq. (2.4); there are additional terms which fall off as powers of $1/r$ and which may in fact dominate over the r^{-L} term. These additional terms have their origin in the fact that one cannot entirely neglect a long range potential no matter how large one chooses r. To prove

this, we note that the Schroedinger equation for angular momentum L with

$$(2\mu/\hbar^2)V(r) = -\beta_n{}^2/r^n$$

has as its two independent solutions

$$r^{\frac{1}{2}} J_{(2L+1)/(n-2)}(x) \text{ and } r^{\frac{1}{2}} N_{(2L+1)/(n-2)}(x)$$

where J and N are cylindrical Bessel and Neumann functions, respectively, and

$$x = 2\beta_n r^{-\frac{1}{2}(n-2)}/(n-2).$$

From the asymptotic forms of these solutions, it follows that the leading terms in the asymptotic form of $u_o(r)$ are, for $n > 2L+3$, r^{L+1} and r^{-L}, just as for a short range potential; one then obtains the usual energy dependence $\eta(L) \to \text{const } k^{2L+1}$ for $k \to 0$. If however $n < 2L+3$, the leading terms in the asymptotic form of $u_o(r)$ are r^{L+1} and r^{L-n+3}, which is not of the usual form, since the latter term dominates the usual r^{-L} term. One does not then have $\eta(L) \to \text{const } k^{2L+1}$ for $k \to 0$, that is, A(L) as defined by Eq. (2.3) does not exist. For $n = 2L+3$, the leading terms in the asymptotic form of $u_o(r)$ are r^{L+1} and r^{-L} $\ell n\ r$, and once again A(L) as defined by Eq. (2.3) does not exist. In this last case, incidentally, one has in the Born approximation that $\eta(L) \to \text{const } k^{2L+1}\ \ell n\ k$, and not simply the k^{2L+1} dependence that has been given in the literature.

A quite different proof of the fact that A(L) as defined by Eq. (2.3) does not always exist follows from the variational expression for A(L) which, in the present notation, takes the form

$$A(L) \approx A_t(L) - [(2L+1)!!]^2 \int u_t(r) \left[\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} - \frac{2\mu}{\hbar^2} V(r)\right] u_t(r)dr, \quad (2.5)$$

where the trial function u_t here satisfies the boundary conditions

$$u_t(0) = 0,\ u_t(r) \to -r^{L+1} + (2L+1)!!(2L-1)!!A_t(L)/r^L.$$

If A(L) does exist the variational expression, Eq. (2.5), should give a value arbitrarily close to A(L) for sufficiently accurate trial functions u_t. However, for any trial function, no matter how accurate, the integrand in Eq. (2.5) approaches $(-2\mu/\hbar^2)V(r)r^{2L+2}$. It follows that if $-2\mu/\hbar^2 V(r) \to \beta_n{}^2/r^n$ for large r the integral is infinite if $2L+2-n \geq -1$. For such values of n and L, then, A(L), as defined by Eq. (2.3), does not exist, in agreement with the conclusion arrived at above.

Recently a number of authors[6-9] have applied the Born approximation to determine the low energy behavior of the phase shift for scattering by long range potentials. To justify this procedure it is usually stated that due to the presence of the centrifugal barrier the low energy scattering is determined only by the asymptotic form of V(r), where V(r) is very weak, the contribution to tan η from zero to any finite value of r going to zero as k^{2L+1}. One might then expect that, for L sufficiently large, the Born approximation will not only give the correct k dependence of the leading term in the expansion of tan η for small k but will also give the correct coefficient of that term. One can go even further. It is almost certainly true that the leading terms in the Born expansion, where only the long range part of V(r) need be taken into account, will give exact results for all terms up to but not including the term in k^{2L+1}. (It should not be difficult to prove this but we have not attempted to do so.) The above expectation is strengthened by the results of the present paper which show by an entirely different approach that they are valid for the particular case n = 4. (Actually, the present paper includes all terms through k^{2L+3}.)

B. Conditions for existence of r_o

If A(L) does not exist, the question of the existence of $r_o(L)$ as defined by Eq. (1.2) does not arise. If A(L) does exist, we must still examine the conditions under which $r_o(L)$ will also exist. We will restrict ourselves to the case L = 0 and to $n \geq 4$. (It should not be very difficult to do the same for $L > 0$.) To analyze the existence conditions, it will be useful to very briefly review effective range theory for short range potentials. Of the derivations of the theory that have been given[1,2], that of Bethe will be most convenient for our present purposes.

Since we are concerned with L = 0, our boundary conditions, Eq. (2.2) and (2.4), become

$$u(0) = 0, \quad u(r) \to \cot \eta(0) \sin kr + \cos kr \tag{2.2}'$$

$$u_o(0) = 0, \quad u_o(r) \to 1 - r/A. \tag{2.4}'$$

We also introduce the solutions of the free Schroedinger equation, with wave numbers k and 0, to be denoted by v(r) and $v_o(r)$, respectively, with normalizations chosen so that they asymptotically approach u(r) and $u_o(r)$, respectively. We then have, for all r,

$$v(r) = \cot \eta(0) \sin kr + \cos kr \tag{2.6}$$

$$v_o(r) = 1 - r/A. \tag{2.7}$$

One can then readily derive the identity

$$k \cot \eta(0) = -(1/A) + k^2 \int_0^\infty (vv_o - uu_o)dr. \tag{2.8}$$

At this stage, an approximation is made. It is argued that if V(r) effectively vanishes for $r > R$, then v is effectively equal to u and v_o to u_o for $r > R$, so

that the integrand is non-negligible only in the region 0 to R. It follows that for $\hbar^2k^2/(2\mu)$ small compared to some average value $\bar{V}$ of V(r) in the region 0 to R, one can, with an error of the order of $k^2\hbar^2/(2\mu\bar{V})$, replace v by v_o and u by u_o in the integrand. We thereby obtain the shape independent approximation, Eq. (1.2), with an error which is presumably proportional to k^4. The energy independent effective range, r_o, is then defined by

$$\tfrac{1}{2}\, r_o = \int_o^\infty (v_o^2 - u_o^2)dr.$$

We have already seen that the shape independent approximation is totally wrong for a repulsive potential equal to a multiple of $1/r^2$. The origin of the error is there clear; a solution $u_o(r)$ which satisfies the boundary conditions given by Eq. (2.4)' does not exist, so that one cannot actually derive the identity, Eq. (2.8), for this case. For potentials which fall off at least as rapidly as $1/r^4$, the identity, Eq. (2.8), is valid. For those cases for which r_o does not exist, the origin of the difficulty must then lie in the subsequent approximations which were made in arriving at Eq. (1.2). The root of the trouble is that the asymptotic form of $u_o(r)$ contains terms in r, r^o, and $r^{-(n-3)}$, (we have $n \geq 4$), while $v_o(r)$ contains only the r and r^o terms. Since $v_o^2 - u_o^2$ will then contain a term of the form $1/r^{n-4}$, it follows that the integral which defines r_o is infinite for n = 4 or 5, that is, that r_o does not exist for n = 4 or 5.

For the case of primary interest, $V(r) \to -\tfrac{1}{2} Z^2e^2 \alpha/r^4$, one has, for example,

$$u_o(r) \to (r/\beta)\sin(\beta/r) - (r/A)\cos(\beta/r)$$

$$= 1 - r/A + \tfrac{1}{2}\beta^2/(Ar) - \beta^2/(6r^2) + \ldots \qquad (2.9)$$

for $r \to \infty$, where

$$\beta^2 = (2\mu/\hbar^2)(\tfrac{1}{2} Z^2 e^2 \alpha). \tag{2.10}$$

Since $v_o(r) = 1 - r/A$ for all r, we have that while $\int_o^\infty (vv_o - uu_o)dr$ is a finite number, the integral which presumably approximates it, namely $\int_o^\infty (v_o^2 - u_o^2)dr$, is infinite.

For those cases for which r_o is infinite, the point then is that while $v_o(r)$ approaches $u_o(r)$ for $r \to \infty$ in the sense that the difference goes to zero, it does not approach it rapidly enough, and there is no point beyond which the effect of the long range potential can be neglected. In fact, returning to the case of arbitrary L, there will for <u>any</u> finite n be <u>some</u> term at which the expansion of $k^{2L+1} \cot \eta(L)$ as a power series in k^2 will break down. On the other hand, if $V(r) \to 0$ for $r \to \infty$ more rapidly than any power of $1/r$, then $v_o(r) - u_o(r) \to 0$ for $r \to \infty$ more rapidly than any power of $1/r$ and the expansion will exist for all L.

3. MATHEMATICAL SOLUTIONS OF SCHROEDINGER EQUATION WITH r^{-4} TERM

In preparation for the derivation of an effective range formula for a potential which approaches a multiple of $1/r^4$ for large r, we seek two independent solutions of the differential equation

$$\left[\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + \frac{\beta^2}{r^4} + k^2\right] G(r) = 0. \tag{3.1}$$

Since we have allowed the term β^2/r^4 to extend all the way in to the origin, we cannot expect either of the two solutions to be a physically acceptable wave function; they will turn out to have a derivative at the origin whose value is not well defined. There cannot be any objection to such a procedure, however, since the solutions are not supposed to represent any physical situation but rather are simply useful mathematical constructs.

One could of course avoid the question by introducing an alternate differential equation in which the $1/r^4$ term is cut off at some small value of r. This would have the further advantage that this potential would correspond more closely to the true potential. On the other hand, it complicates the mathematics, and since the introduction of Eq. (3.1) does not lead to any difficulties, we prefer to use that approach.

Following Vogt and Wannier[10], we introduce the new variable Z and the new function $\phi(Z)$ through

$$r = (\beta/k)^{\frac{1}{2}} e^{Z} \tag{3.2}$$

and

$$G(r) = r^{\frac{1}{2}} \phi(Z). \tag{3.3}$$

$\phi(Z)$ then satisfies the Mathieu equation,

$$\left[\frac{d^2}{dZ^2} - (L + \tfrac{1}{2})^2 + 2\beta k \cosh(2Z)\right]\phi(Z) = 0; \tag{3.4}$$

the properties of the solutions of this equation are rather well known[11]. Reverting to the co-ordinate r, the two independent solutions can be taken to be

$$M_{\pm\nu}^{(1)} = M_{\pm\nu}^{(1)} \left\{ \ell n\left[(\beta/k)^{-\frac{1}{2}} r\right] \right\}, \tag{3.5}$$

where, to lowest orders in βk, one has[12]

$$\nu \approx (L + \tfrac{1}{2}) - (\beta k)^2 \Big/ \left[4(L + \tfrac{3}{2})(L + \tfrac{1}{2})(L - \tfrac{1}{2})\right]. \tag{3.6}$$

It will also be convenient to introduce the quantities

$$m \equiv M_{\nu}^{(1)}(0) \Big/ M_{-\nu}^{(1)}(0) \tag{3.7}$$

and

$$\delta \equiv \tfrac{1}{2}\pi(\nu - L - \tfrac{1}{2}) \approx -\pi\beta^2 k^2 \Big/ \left[8(L + \tfrac{3}{2})(L + \tfrac{1}{2})(L - \tfrac{1}{2})\right]. \tag{3.8}$$

m can be expanded as

$$m = (\tfrac{1}{4}\beta k)^{\nu} \left[\Gamma(1 - \nu)/\Gamma(1 + \nu)\right]\left[1 + C_1\beta^2 k^2 + C_2\beta^4 k^4 + \ldots\right], \tag{3.9}$$

where C_1 and C_2 follow from an analysis of Eqs. (2.6-22) and (2.2-38) of reference 11, and where Γ is the gamma function. The leading term of Eq. (3.9) is given explicitly by

$$m = (-1)^L(2L+1)(\beta k)^{L+\frac{1}{2}} \Big/ \left[(2L+1)!!\right]^2 + \ldots \tag{3.10}$$

while the next term follows from the relationship

$$C_1 = -\tfrac{1}{4}\nu/(1 - \nu^2)^2. \tag{3.11}$$

For our purposes, it will be convenient to choose as the two independent solutions

$$v_{ps}(r) = Q\left[m \cos\delta\, M_{-\nu}^{(1)} + (-1)^L(1/m)\sin\delta\, M_{\nu}^{(1)}\right], \tag{3.12}$$

and

$$v_{pc}(r) = Q\left[m \sin\delta\, M_{-\nu}^{(1)} + (-1)^L (1/m) \cos\delta\, M_{\nu}^{(1)}\right], \tag{3.13}$$

where

$$Q \equiv (\tfrac{1}{2}\pi/\beta)^{\frac{1}{2}}\, r^{\frac{1}{2}} \Big/ \cos 2\delta. \tag{3.14}$$

The subscript p refers to the fact that the differential equation under consideration contains the polarization potential. The subscripts s and c are suggested by the sine and cosine dependence of the functions for sufficiently small r. Thus, it follows from the known properties of the $M_{\pm\nu}^{(1)}$ that

$$v_{ps}(r) \sim \sin\left[(\beta/r) - \tfrac{1}{2}L\pi\right] \Big/ (\beta/r), \qquad r \ll (\beta/k)^{\frac{1}{2}},$$

$$v_{pc}(r) \sim \cos\left[(\beta/r) - \tfrac{1}{2}L\pi\right] \Big/ (\beta/r), \qquad r \ll (\beta/k)^{\frac{1}{2}}.$$

For large r, we have

$$v_{ps}(r) \sim \frac{(-1)^L m}{(\beta k)^{\frac{1}{2}} \cos 2\delta}\left[\cos(kr - \tfrac{1}{2}L\pi)\left(\cos^2\delta - \frac{\sin^2\delta}{m^2}\right)\right.$$

$$\left. + \sin(kr - \tfrac{1}{2}L\pi)\sin\delta\cos\delta\left(\frac{1}{m^2} - 1\right)\right], \qquad r \gg (\beta/k)^{\frac{1}{2}} \tag{3.15}$$

$$v_{pc}(r) \sim \frac{(-1)^L m}{(\beta k)^{\frac{1}{2}} \cos 2\delta}\left[\cos(kr - \tfrac{1}{2}L\pi)\sin\delta\cos\delta\left(1 - \frac{1}{m^2}\right)\right.$$

$$\left. + \sin(kr - \tfrac{1}{2}L\pi)\left(\frac{\cos^2\delta}{m^2} - \sin^2\delta\right)\right], \qquad r \gg (\beta/k)^{\frac{1}{2}}. \tag{3.16}$$

As for short range potentials, the two independent solutions have been chosen in such a way as to make their behavior for small r relatively simple. There is no need to choose solutions which have a simple behavior at large r since the u(r) and v(r) are chosen to approach one another at large r and one never actually has to perform calculations with the functions at large r.

4. MODIFIED EFFECTIVE RANGE EXPANSION

In our analysis of Eq. (2.1) for short range potentials, we took u(r) at large r to be a linear combination of the two solutions of that equation with V(r) neglected, i.e., kr $j_L(kr)$ and kr $n_L(kr)$. The relative amplitude of these two terms, which is fixed by the requirement that the continuation of u(r) must vanish at r = 0, determines the phase shift. We are now however concerned with a long range potential such that

$$\Delta V(r) \equiv V(r) + (\hbar^2/2\mu)\, \beta^2/r^4 \tag{4.1}$$

vanishes as $r \to \infty$ more rapidly than any power of 1/r. A modified approach must then be used if we are to obtain the equivalent of an effective range expansion, for we have seen that r_o as normally defined does not exist. We rewrite our differential equation as

$$\left[\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + \frac{\beta^2}{r^4} - \frac{2\mu}{\hbar^2}\Delta V(r) + k^2\right] u(r) = 0.$$

Since $\Delta V(r)$ <u>is</u> a short range potential, we can neglect it at large r, and write u(r) as a linear combination of the solutions of the resultant equation, namely, v_{ps} and v_{pc}. The relative amplitude, which we will denote by B, can readily be related to tan $\eta(L)$.

Thus, we solve the differential equation, Eq. (2.1), subject to the boundary conditions

$$u(0) = 0, \; u(r) \to v_{ps}(r) + B\, v_{pc}(r). \tag{4.2}$$

Once B has been found, $\tan \eta(L)$ is determined, since inserting the asymptotic forms of v_{ps} and v_{pc}, and comparing with the usual asymptotic form $u(r) \to \text{const} \times \sin\left[kr - \frac{1}{2} L\pi + \eta(L)\right]$, one finds

$$\tan \eta(L) = \frac{m^2 - \tan^2\delta + B \tan \delta(m^2-1)}{\tan \delta(1-m^2) + B(1-m^2 \tan^2\delta)} . \tag{4.3}$$

For the development of a modified effective range theory, it is useful to define

$$v_p(r) = v_{ps}(r) + B\, v_{pc}(r) \tag{4.4}$$

for all r. We then let $u_1(r)$ and $u_2(r)$ be solutions of Eq. (2.1) for energies E_1 and E_2, respectively, and $v_{p1}(r)$ and $v_{p2}(r)$ be the corresponding solutions of Eq. (3.1); all four solutions satisfy the appropriate boundary conditions. Proceeding then in a fashion almost identical with that used by Bethe[2], we find

$$\left(u_1 u_2' - u_2 u_1'\right)\Big|_a^b = (k_1^2 - k_2^2) \int_a^b u_1 u_2 \, dr,$$

$$\left(v_{p1} v_{p2}' - v_{p2} v_{p1}'\right)\Big|_a^b = (k_1^2 - k_2^2) \int_a^b v_{p1} v_{p2} \, dr, \tag{4.5}$$

where a and b are arbitrary. Subtracting, letting $a \to 0$ and $b \to \infty$, and using the specified forms of the various functions and their derivatives

for very small and for very large values of r, we obtain

$$(B_2/\beta) - (B_1/\beta) = (k_2^2 - k_1^2) \int_0^\infty (v_{p2}v_{p1} - u_2u_1)dr. \qquad (4.6)$$

Eq. (4.6) is valid for all L. The situation in the present case is then in this regard simpler than than for a short range potential, where the derivation of an effective range expansion is rather different for $L > 0$ than for $L = 0$, the difference arising due to the presence of the $L(L+1)/r^2$ terms which give rise to difficulties at $r = 0$ for $L > 0$. For our present long range potential, the $1/r^4$ term dominates the $L(L+1)/r^2$ for $r \to 0$ for all L, so one need not distinguish between $L = 0$ and $L > 0$. Note that the identity, Eq. (4.6), reduces for $L = 0$ to that deduced by Bethe for $\beta \to 0$. That it does so follows from the observation that $B/\beta \to k \cot \eta(0)$ for $\beta \to 0$.

The long range polarization effects having been accounted for, the difference between v_{p1} and u_1, or between v_{p2} and u_2, falls off faster than any power of $1/r$. It was precisely because the difference between u_1 and v_1 or between u_2 and v_2 did <u>not</u> fall off faster than any power of $1/r$, for the conventional form for v_1 or for v_2, that the effective range expansion for $k^{2L+1} \cot \eta(L)$ broke down. We <u>do</u> however have a valid effective range expansion for B/β.

5. EXPANSION ABOUT ZERO ENERGY

We specialize now to the case for which $E_1 = 0$. Denoting the corresponding quantities by the subscript o, we then have

$$v_{po}(r) = j_L(\beta/r) - B_o n_L(\beta/r). \tag{5.1}$$

Dropping the subscript 2, Eq. (4.6) becomes

$$(B/\beta) = (B_o/\beta) + \tfrac{1}{2}\rho_p(0,E)k^2, \tag{5.2}$$

where

$$\tfrac{1}{2}\rho_p(0,E) \equiv \int_o^\infty (v_{po}v_p - u_o u)dr. \tag{5.3}$$

Thus far, all of our equations are exact. We now write[13]

$$(B/\beta) \approx (B_o/\beta) + \tfrac{1}{2} r_{po}k^2, \tag{5.4}$$

where

$$\tfrac{1}{2} r_{po} \equiv \tfrac{1}{2}\rho_p(0,0) = \int_o^\infty (v_{po}^2 - u_o^2)dr, \tag{5.5}$$

and where the error involves a term of order k^4, the relative error being of the order of $(h^2k^2/2\mu)/\bar{V}$; here $\bar{V}$ is some average value of V(r) taken over the range of the short range potential.

From Eq. (4.3) we find that

$$\lim_{k\to o} (\tan \eta(0)/k) \equiv -A = \beta/B_o. \tag{5.6}$$

Using Eqs. (2.3), (3.8), (3.9), and (4.3), Eq. (5.4) can be written, to terms in k^2, as

$$k \cot \eta(0) = -\frac{1}{A} + \frac{\pi\beta^2}{3A^2} k + \frac{4\beta^2}{3A} k^2 \ell n(\tfrac{\beta k}{4}) + \left[\tfrac{1}{2}r_{po} + \frac{\pi\beta}{3} + \frac{20\beta^2}{9A} - \frac{8\beta^2}{3A}\psi(\tfrac{3}{2}) - \frac{\pi\beta^3}{3A^2} - \frac{\pi^2\beta^4}{9A^3}\right]k^2 + \ldots, \tag{5.7}$$

where

$$\psi(\tfrac{3}{2}) = \Gamma'(\tfrac{3}{2})/\Gamma(\tfrac{3}{2}) = 0.0365.$$

The expansion for tan $\eta(0)$ is slightly simpler in form. We have given the expansion for k cot $\eta(0)$ simply because that is the conventional form.

It is well known that k cot $\eta(0)$ must be an even function of k for real k. This property does not depend upon any special properties of V(r), contrary to the situation when one is attempting to prove the analyticity of k cot $\eta(0)$. Despite the appearance of Eq. (5.7), k cot $\eta(0)$ is in fact an even function of k. The point is that for k real and negative, one must utilize an alternate asymptotic expansion of the Mathieu functions[14], and it is found that in Eq. (5.7) k must everywhere be replaced by -k.

For a potential V(r) for which $\Delta V(r)$ as defined by Eq. (4.1) vanishes more rapidly than any power of 1/r, as we have assumed, one could obtain the coefficient of k^3 in the expansion of k cot $\eta(0)$ without introducing any new parameters; the coefficient is in fact independent of r_o and can be expressed in terms of A and β. In most cases of interest, however, $\Delta V(r)$ will have additional terms that vanish as d/r^6, and the coefficient will then depend upon d as well. We have therefore not calculated the k^3 term. We will not here go into this point any further.

The term linear in k in Eq. (5.7) has previously been found by Thaler[8] in a Born approximation analysis of the effect of the polarizability of the neutron on the scattering of neutrons by nuclei with large Z.

For $L > 0$, Eq. (4.3) leads to

$$\tan \eta(L) = -\tan \delta + (2L+1)(\beta k)^{2L+1}\left[(2L-1)!!\right]^{-2} B_o^{-1}. \qquad (5.8)$$

[This equation is in fact valid for L = 0 as well, but for that case we have gone well beyond this result in Eq. (5.7).] Higher order terms in the expansion of δ, (see Eq. (3.8)), can be obtained. The expansion of tan $\eta(L)$ up through terms not including k^{2L+1} can then be expressed in terms of β alone, while the expansion including the k^{2L+1} term involves in addition only B_o. The k^{2L+1} term is of course the leading term for short range potentials.

It should be noted that the techniques previously[15] introduced for short range potentials for the determination of rigorous upper bounds on $A(L)$ can readily be adapted to determine rigorous upper bounds on $-1/B_o$. One would use the normalization

$$u_o(r) \to n_L(\beta/r) - (1/B_o) j_L(\beta/r).$$

The leading term in the above expansion is given by

$$\tan \eta(L) = \left\{ \pi\beta^2 \Big/ \left[8(L + \tfrac{3}{2})(L + \tfrac{1}{2})(L - \tfrac{1}{2}) \right] \right\} k^2 + \ldots$$

That $\eta(L)$ is proportional to k^2 and not to k^{2L+1} for k sufficiently small and $L > 0$ has previously been shown to be true in the Born approximation[7,8]. Thaler in fact found the above coefficient for L = 1 and L = 2.[16]

It might be noted that to lowest order in k, the total cross section is now given by the expression

$$\sigma = 4\pi A^2 + (8/3)\pi^2\beta^2 Ak + \ldots$$

We have throughout the paper expressed all expansions in terms of β, B_o, and r_{po}. In many ways, it would be preferable to determine the expan-

sion in terms of B_o, r_{po}, and the various quantities connected with the Mathieu solutions, such as ν, m, and δ, without expanding these latter quantities as power series in k^2, since these quantities are rather delicate functions of k. For a polarizability numerically equal to that of a Hydrogen atom, the expansions break down in the neighborhood of 1.5 ev. For scattering by a compound system, where one is dealing with a partial differential equation, it would be perfectly reasonable to determine the quantities ν, m, and δ, which are defined by an ordinary differential equation, numerically, and to proceed from there. With this point of view, the potential which goes as $1/r^4$ is no simpler than other long range potentials.

The limitation to energies below about 1.5 ev, for β equal to that of a Hydrogen atom, might seem to be severe. On the other hand, this is easily the energy interval most difficult to study, both theoretically and experimentally. Furthermore, the adiabatic approximation on which the $1/r^4$ potential is based cannot be valid at any but very low energies, though precisely how low is not really known. Thus, it does not seem worthwhile to seek alternate expansions of ν, m, and δ which are valid for higher energies, even though they must exist, or even to seek numerical values of ν, m, and δ in the higher energy range.

6. EXPANSION ABOUT ENERGY OF BOUND STATE

If there exists a bound state of angular momentum L with energy $E_\gamma = -\hbar^2\gamma^2/(2\mu)$ which is very small and which is known, it is well known in the usual effective range theory that it is often more convenient to expand about $E = E_\gamma$ rather than about $E = 0$. The same is true for the

present case of a long range potential, though here we will be concerned initially with the expansion of B and only then with the expansion of cot $\eta(L)$.

Thus, while Eq. (4.6) was derived for two non-negative energies, it remains valid when one of the energies is negative, and when both of the energies are negative. The point is that the expressions for the Mathieu functions that were used in the derivation of Eq. (4.6) are valid not simply for k real and positive but rather in the sector $-\pi < \arg k < \pi$. (We make specific note of the fact that the expressions are not valid for k real and negative. This point was critical in the proof that $\eta(L)$ is an odd function of k.) Eq. (4.6) can then be written as

$$(B/\beta) = (B_\gamma/\beta) + (k^2 + \gamma^2) \int_0^\infty (v_{p\gamma} v_p - u_\gamma u) dr. \tag{6.1}$$

Proceeding in a fashion identical to that used at zero energy, this identity can be approximated by

$$(B/\beta) \approx (B_\gamma/\beta) + \tfrac{1}{2} \rho_{p\gamma} (k^2 + \gamma^2) \tag{6.2}$$

where the energy independent effective range, $\rho_{p\gamma}$, is defined by

$$\tfrac{1}{2} \rho_{p\gamma} \equiv \int_0^\infty (v_{p\gamma}^2 - u_\gamma^2) dr. \tag{6.3}$$

One advantage of the present expansion about $E = E_\gamma$ over the expansion about $E = 0$ is that whereas B_o depended upon $V(r)$ for small r in a detailed way, B_γ follows immediately simply from a knowledge of E_γ, and E_γ will often be known experimentally. Thus the requirement that the bound state function

behave asymptotically like $e^{-\gamma r}$ leads [see Eqs. (3.15), (3.16), and (4.2), replacing k by $i\gamma$] to the expression

$$B_\gamma = \frac{im_\gamma^2 e^{2i\delta_\gamma} - \tan \delta_\gamma}{1 + im_\gamma^2 e^{2i\delta_\gamma} \tan \delta_\gamma} \tag{6.4}$$

where m_γ and δ_γ are to be evaluated at $E = E_\gamma$.[17] Specializing now to the particularly important case of L = 0, we have

$$\delta_\gamma = -\tfrac{1}{3}\pi\beta^2\gamma^2 + \ldots \qquad \text{for } L = 0 \tag{6.5}$$

and

$$im_\gamma^2 e^{2i\delta_\gamma} = \beta\gamma + O(\gamma^3 \ln \gamma) \quad \text{for } L = 0 \tag{6.6}$$

so that, to terms in γ^2,

$$B_\gamma \approx -\beta\gamma + \tfrac{1}{3}\pi\beta^2\gamma^2 , \qquad \text{for } L = 0. \tag{6.7}$$

From Eqs. (3.8), (3.11), (4.3), (6.2), and (6.7), one then finds

$$k \cot \eta(0) \approx -\gamma + (\tfrac{1}{2}\rho_{p\gamma} + \tfrac{1}{3}\pi\beta)(\gamma^2 + k^2). \tag{6.8}$$

Eq. (6.8) differs from the usual expansion in that it contains $\frac{1}{2}\rho_{p\gamma} + \frac{1}{3}\pi\beta$ rather than $\frac{1}{2}\rho_\gamma$. We will now show that to the order to which we are working, these two expressions are the same.

Thus, consider the function $v_{p\gamma'}$, which is defined by the same differential equation and boundary conditions which determine $v_{p\gamma}$ except that γ is replaced by γ'. (We do not assume the existence of a bound state with energy $(\hbar^2/2\mu)\gamma'^2$.) By manipulating the two differential equations for $v_{p\gamma}$ and $v_{p\gamma'}$, we obtain, in the usual way,

$$(\gamma^2 - \gamma'^2) \int_0^\infty v_{p\gamma} v_{p\gamma'} dr = (v_{p\gamma'} v_{p\gamma}' - v_{p\gamma} v_{p\gamma'}')\Big|_0^\infty$$

$$= -(1/\beta)(B_\gamma - B_{\gamma'}).$$

If we let γ' approach γ the desired integral may be written

$$\int_0^\infty v_{p\gamma}^2 dr = -\frac{1}{\beta} \frac{dB_\gamma}{d\gamma^2} = -\frac{1}{2\beta\gamma} \frac{dB_\gamma}{d\gamma} \approx \frac{1}{2\gamma} - \tfrac{1}{3}\pi\beta.$$

It follows that

$$\tfrac{1}{2}\rho_{p\gamma} \approx 1/(2\gamma) - \tfrac{1}{3}\pi\beta - \int_0^\infty u_\gamma^2 \, dr. \tag{6.9}$$

On the other hand, since $v_\gamma = \exp(-\gamma r)$, we have

$$\tfrac{1}{2}\rho_\gamma \equiv \int (v_\gamma^2 - u_\gamma^2) dr = 1/(2\gamma) - \int_0^\infty u_\gamma^2 \, dr. \tag{6.10}$$

Eq. (6.8) can therefore be written as

$$k \cot \eta(0) \approx -\gamma + \tfrac{1}{2}\rho_\gamma(\gamma^2 + k^2). \tag{6.11}$$

Thus, to order γ^2, the formulation which explicitly takes into account the long range character of the potential leads to precisely the same result as the usual formulation utilized in application to short range potentials. This conclusion must still, of course, be verified for scattering by a compound system when identical particles are involved. Furthermore, even if the ordinary shape-independent formula is valid in this case, it is

very unlikely that the error term is of order k^4 since in the one body problem one does find lower order corrections. With these qualifications, our results then justify the very nice use which has been made of Eq. (6.11) in the analysis of low energy singlet scattering of electrons by Hydrogen atoms,[18] and makes less surprising the good agreement obtained between the singlet scattering length thereby obtained and that determined on the basis of a rigorous minimum principle.[19]

It is of interest to inquire into the absence of a term linear in k (as well as a number of other terms) in the present expansion about $E = E_\gamma$ as contrasted to the situation of the expansion about $E = 0$. This can be discussed in a number of ways. On the one hand, we saw that the integral which defined ρ_o did not even exist, due to the difference in the asymptotic behavior of v_o and of u_o; while v_γ and u_γ also have a different asymptotic behavior, they are both now dominated by the factor $e^{-\gamma r}$, so that $\int v_\gamma^2 dr$ and $\int u_\gamma^2 dr$ exist separately, and hence so does ρ_γ. More physically, one can understand the difference in the following way. In the expansion about $E = 0$, no assumption whatever was made about the magnitude of A and only terms in k^3 were neglected. The expansion about $E = E_\gamma$ assumes however that E_γ and hence γ is small, and terms in γ^3, $\gamma^2 k$, and γk^2 were neglected, as well as terms in k^3. Now it follows from a comparison of the two expansions of $k \cot \eta(0)$, about $E = 0$ and about $E = E_\gamma$, that $1/A$ is small if γ is small. (In fact, $1/A \approx \gamma$.) If in Eq. (5.7) we drop terms in $1/A^3$, in (k/A^2), and in (k^2/A), which are now on the same footing as k^3 terms, we remain with

$$k \cot \eta(0) \approx -1/A + (\tfrac{1}{2} r_{po} + \tfrac{1}{3} \pi\beta)k^2 \approx -1/A + \tfrac{1}{2} r_o k^2,$$

which is just the usual expansion. On the other hand, no matter how small $1/A$ is, there will always be an interval in the neighborhood of $k = 0$, a very small interval to be sure, for which the term linear in k will be more important than the terms in $k^2 \ln k$ and in k^2.

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[2] H.A. Bethe, Phys. Rev. 76, 38 (1949).

[3] With the exception of the spherical Bessel functions $j_L(kr)$ and $n_L(kr)$, the angular momentum under consideration, when explicitly indicated, will appear in parentheses; subscripts will generally refer to the energy under consideration.

[4] The smallness of the numerical value of some characteristic length, which is after all a dimensional quantity, is not necessarily a measure of the usefulness of effective range theory. Energies are in many regards "scaled" in relation to the characteristic length, and it is probably true that in general the range of validity of effective range theory will cover a significant portion of the energy spectrum. It seems fair to say that effective range theory was introduced in nuclear rather than in atomic theory not because of the disparity in the values of the characteristic lengths but because of the lack of knowledge of the nuclear potential. To the extent that the nuclear potential can now be considered to be known, and to the extent that we restrict ourselves to scattering by a compound system - these are of course very severe restrictions - effective range theory, appropriately modified, is potentially as valuable in atomic as in nuclear physics.

[5] A preliminary discussion of the results of the present paper has already appeared. [L. Spruch, T.F. O'Malley, and L. Rosenberg, Phys. Rev. Letters 5, 375 (1960)]. Eq. (1) of this reference contains a misprint; in the last term on the right hand side A^2 should be replaced by A^3.

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$$\beta = \nu - L, \quad \cos \pi\gamma = (1 + m^2)/(2m),$$

$$e^{\phi} = (-1)^L(1 - m^2)/(2m \sin \nu\pi).$$

[11] J. Meixner and F.W. Schafke, Die Grundlehren der Mathematischen Wissenschaften, (Springer-Verlag, Berlin, 1954), Vol. 71.

[12] The higher terms in the expansion of ν can be obtained from the expansion of cos $\nu\pi$ given by Meixner and Schafke, reference 11, Eq.(2.2-44).These higher terms will not however be required for our present purposes.

[13] Eq. (5.4) is identical in form with the usual expansion for k^{2L+1} cot $\eta(L)$, v_p having been chosen to accomplish this. Eq. (4.3) is then rather more complicated in form than it might otherwise be.

[14] The alternate asymptotic expansion of the Mathieu function follows from the realization (see reference 11) that $M_\nu^{(1)}$ approaches J_ν, and that there are different asymptotic expansions of J_ν depending upon which sector of the complex plane the argument of J_ν lies in.

[15] L. Spruch and L. Rosenberg, Phys. Rev. 116, 1034 (1959); 117, 1095 (1960) and L. Rosenberg, L. Spruch, and T.F. O'Malley, Phys. Rev. 118, 184 (1960).

[16] Thaler's expression[8] for arbitrary L is correct only for L = 1 and for L = 2.

[17] The replacement of k by ik is permissible because, as noted previously, the Mathieu functions that we have used are valid for $-\pi < \arg k < \pi$; the question of the analyticity of k cot $\eta(L)$, for example, does not arise. Eq. (6.4), incidentally, is formally equivalent to replacing tan $\eta(L)$ by i in Eq. (4.3).

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